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On statistical mechanics of non-equilibrium phenomena

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Introduction

The present work is an attempt to develop a consistent framework for the description of non equilibrium phenomena on the basis of statistical mechanics (classical or quantal). For this purpose a phase space is constructed whose points (elementary events) are the possible outcomes of an experiment which consists of the "continuous" measurement of certain macroscopic observables. This phase space possesses a "natural" measure, corresponding to the Liouville measure in classical mechanics. In general the "natural" measure is infinite. The equations of motion generate a group, parametrized by the time, of point transformations which preserve the "natural" measure. The constructed phase space of the experiment is hence formally analogous to the phase space of classical mechanics but contrary to this space it is composed entirely of macroscopically observable elements. The analogy to the classical phase space is further stressed by the existence of a "time reversal" transformation which preserves the "natural" measure. In the same way as the classical phase space is decomposed into energy surfaces and possibly further invariant subregions, the phase space of the experiment is decomposed into ergodic classes of finite measure, corresponding to different values of certain "integrals of the macroscopic motion". One of these is the macroscopic energy. The integrals of the macroscopic motion characterize the macroscopic conditions under which a given experiment is carried out, in particular they determine the macroscopic equilibrium state which is possibly reached. The phase space structure of the experiment can be said to be equivalent to a class of stochastic processes which are stationary, ergodic, and satisfy time reversal symmetry. Each stationary stochastic process of the class describes the fluctuations of the macroscopic observables in a given equilibrium state. The approach to equilibrium from an arbitrary initial state is described by the corresponding conditional stochastic process, which is determined by the stationary process.

The construction of the phase space of the experiment must be based on a prescription for the interpretation of (ideal) macroscopic observations on a microscopic level. It is wellknown that von Neumann [von Neumann, 1932 a] has given a prescription of how the quantum mechanical state or rather the density operator is changed when a non sharp observable is measured and that his point of view has been criticized by Lüders [Lüders, 1951] and others. It is sometimes erroneously proposed that the change of state by measurement is a sort of physical procedure peculiar to quantum theory, which possibly could be considered as the source of macroscopic irreversibility. In reality we are here dealing with a logical procedure which has a complete classical analogue, the construction of a conditional probability distribution. With this fact in mind we find it necessary to attach ourselves to Lüders' criticism of von Neumann's prescription.

The phase space structure of an experiment is developed in the first four sections and the rest of the paper is concerned with a study of the general properties of this structure. In particular questions concerning recurrence and approach to equilibrium are discussed.

1. The energy-structure function

For the purposes of statistical thermodynamics a mechanical system of a finite number of degrees of freedom is sufficiently characterized by its structure function $V(E;\, H)$; $0 \leqslant E < \infty$, the extension-in-phase or the number of energy states below a certain value E of the energy. The notation $V(\,.\,;\, H)$ indicates the functional dependence of the structure function on the Hamiltonian. Equivalently the structure function can be given in term of its Laplace transform, the sum-over-states

$$\exp\{-Y(\beta;\, H)\} = \int_0^\infty \exp\{-\beta E\}\, d_E\, V(E;\, H); \qquad (0 < \beta < \infty), \tag{1}$$

or its negative logarithm $Y(\beta;\, H)$, the Massieu-Planck function, from which the thermodynamic properties of the system are directly obtained. The fundamental problem of statistical thermodynamics is the determination of the structure function for mechanical systems of macroscopic dimensions. If the system can be considered as built up of almost independent parts the Massieu-Planck function of the total system is equal to the sum of the Massieu-Planck functions of its parts and for a system composed of a large number of similar and independent parts the asymptotic form of the structure function can be obtained in a rigorous way by use of the techniques of the central limit theorem of probability [Khinchin, 1949], [Blanc-Lapierre and Tortrat, 1956]. The first result of this kind is due to Maxwell [Maxwell, 1878], who derived the explicit form of the structure function corresponding to the kinetic energy of a system of particles having the same mass. From the exact form of the structure function he obtained its asymptotic form.

It is an almost trivial fact that the existence of the sum-over-states for all positive values of β is a considerable restriction on the types of Hamiltonians considered in statistical thermodynamics. In particular it implies in the quantum mechanical case that the Hermitian operator

$$\exp\{-\beta H\} \tag{2}$$

in the state-vector space, having a finite trace, is compact (completely continuous) and hence has a pure point spectrum, which is either finite or infinite with 0 as its only accumulation point.[1] Each eigenvalue is only finitely degenerated.

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[1] The fact that (2) is compact may also be used as the starting point for a systematic determination of the eigenvalues of H.

In the quantum mechanical case the Stieltjes integral (1) is thus always reduced to a sum, in general infinite. It is important to recall these properties of the Hamiltonian when discussing the dynamics of the system, in particular when going to the limit of "infinitely large" systems.

2. Generalized structure functions

For the purposes of non equilibrium thermodynamics it is sometimes necessary to consider generalizations of the thermodynamic functions corresponding to the equilibrium theory. On a statistical mechanical basis these generalized thermodynamic functions can be obtained from generalized structure functions, [Klein, 1952].

Let the macroscopic observables

$$A=(A^1, \dots, A^n) \tag{3}$$

be associated with the real phase functions, or Hermitian operators

$$a=(a^1, \dots, a^n). \tag{4}$$

We assume that the observables A can be measured together, so that the corresponding operators are compatible. Let

$$i=(i^1, \dots, i^n) \tag{5}$$

be n arbitrary intervals on the real axis. With the interval i^μ and the observable A^μ we associate a phase function $I^\mu(i^\mu)$ which has the value 1 in the phase points corresponding to a value of the phase function a^μ in the interval i^μ and has the value 0 in every other phase point. Or we associate with the interval i^μ the projection operator $I^\mu(i^\mu)$, in the state-vector space, which corresponds to the interval i^μ in the spectral resolution of the operator a^μ. The product

$$I(i)=I^1(i^1)\dots I^n(i^n) \tag{6}$$

is again a function of the phase with values 1 and 0, or a projection operator. The structure function corresponding to the n observables A is defined as a function of the n-dimensional interval i (5):

$$V(i;A)=\mathcal{S}\,I(i) \tag{7}$$

where the symbol $\mathcal{S}$ denotes integration over the phase space with the Liouville-measure $h^{-f}dp_1\dots dq_f$, h denoting Planck's constant and f the number of degrees of freedom, or $\mathcal{S}$ denotes the trace operation. The interval function $V(.;A)$ defines a measure in the n-dimensional Euclidean space R^n which we denote by the same symbol.

Asymptotic expressions for the structure function (7) can be obtained under conditions analogous to those for the energy structure function.[1]

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[1] For a discussion see e.g. [Uhlhorn, 1960 a] where further references are given.

It is clear that the structure function $V(.;A)$ represents only a part of the structure of the mechanical system, namely exactly that part which is determined by the observables A. Thus any question relative to the observables A can be answered with the aid of the function $V(.;A)$, so that if the observables A are the only quantities accessible to observation, the relevant "phase space" of the system is the n-dimensional Euclidean space, with the "natural measure", $V(.;A)$ corresponding to the Liouville measure in the complete classical phase space. The characterization of the system has thus been considerably contracted, corresponding to the coarser description.

3. Repeated observations and the corresponding structure functions

The experimental situation which motivates the introduction of the structure function $V(.;A)$ is the simultaneous measurement of the observables A at *one* single time.

We are, however, very often interested in the comparison of observations made at different times. If for instance we claim that in the course of time a system reaches equilibrium we are referring to the behaviour of a time series of observed values of a macroscopic observable.

From the statistical mechanical point of view we are therefore interested in *all possible* series of observed values corresponding to a given experiment which consists in the observation of a macroscopic observable at prescribed times. It is natural to call the totality of possible series of observed values the phase space of the experiment and to introduce a structure function corresponding to the given experiment.

To make this clear we shall assume that the experiment consists in the determination of the macroscopic observables A at two times $t_1 < t_2$. The result of an experiment can then always be expressed in the form

$$A(t_1) \in i_1; \quad A(t_2) \in i_2 \tag{8}$$[1]

where i_1 and i_2 are n-dimensional intervals (5). The structure function corresponding to observable events of the form (8) will be a function of the $2n$-dimensional interval $i_1 \times i_2$. In order to define it we need the mechanical equations of motion.

3.1. *Classical mechanics*

In the classical case Hamilton's equations generate a group of point transformations $u(.)$ in the phase space Z

$$\zeta_t = u(t)\,\zeta_0; \quad u(t)\,u(t')\,\zeta = u(t+t')\,\zeta; \quad (-\infty < t, t' < +\infty). \tag{9}$$

where ζ denotes the phase point $(p_1, \dots, q_f)$. The point transformations $u(.)$ preserve the Liouville measure $d\zeta = h^{-f}\, d\, p_1 \dots d\, q_f$ (Liouville's theorem).

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[1] The symbol $\in$ denotes "is an element of".

The mechanical system being closed, the equations of motion are invariant under time reversal or properly under reversal of the direction of motion. That is, there exists an involutory transformation τ in the phase space

$$\tau \tau \zeta = \zeta, \tag{10}$$

which preserves the Liouville measure, and is related to the group $u(.)$ of kinetic transformations by

$$\tau u(t) = u(-t) \tau. \tag{11}$$

By the algebra of classical observables we shall understand the system of all complex and bounded functions $x, y, \ldots$ on the phase space[1] with the algebraic operations defined by

$$(\lambda x + \mu y)(\zeta) = \lambda x(\zeta) + \mu y(\zeta), \qquad (\lambda, \mu \text{ complex numbers}), \tag{12}$$

$$(x y)(\zeta) = x(\zeta) y(\zeta). \tag{13}$$

The group of kinetic transformations $u(.)$ induces a group of transformations $U(.)$ of the algebra of classical observables onto itself [Koopman, 1931]

$$U(t) x(\zeta) = x(u(t) \zeta) \qquad (-\infty < t < +\infty). \tag{14}$$

Evidently $U(.)$ is a group of isomorphisms of the algebra

$$\begin{aligned} U(t)(\lambda x + \mu y) &= \lambda U(t) x + \mu U(t) y, \\ U(t)[x y] &= [U(t) x][U(t) y] \end{aligned} \tag{15}$$

which commutes with the *-operation, the taking of the complex conjugate,

$$[U(t) x]^* = U(t) x^*. \tag{16}$$

Further the integral S is invariant under $U(.)$

$$S U(t) x = \int d\zeta \, x(u(t) \zeta) = \int d\zeta \, x(\zeta) = S x,^2 \tag{17}$$

which is equivalent to Liouville's theorem.

The time reversal operator T is defined by

$$T x(\zeta) = x(\tau \zeta) \tag{18}$$

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[1] Properly, we should use the expression essentially bounded with reference to the Liouville measure. The norm of an element x in the algebra, $\|x\|$ is defined as the essential least upper bound of the function $|x(\zeta)|$. The algebra of classical observables is in the mathematical terminology a commutative Banach algebra with a *-operation, the taking of the complex conjugate. The conventional notation for this algebra is $L^\infty(Z, d\zeta)$, Z denoting the phase space.

[2] If x is such that the integral $S x$ has a meaning.

for any classical observable. From the properties of the transformation τ it follows that the time reversal operator is an involution

$$T\,T = 1, \tag{19}$$

an isomorphism of the algebra of classical observables

$$\begin{aligned} T\,(\lambda\,x + \mu\,y) &= \lambda\,T\,x + \mu\,T\,y \\ T\,[x\,y] &= [T\,x]\,[T\,y], \end{aligned} \tag{20}$$

which commutes with the *-operation

$$[T\,x]^* = T\,x^*, \tag{21}$$

and that the integral S is invariant under T

$$S\,T\,x = \int d\,\zeta\,x\,(\tau\,\zeta) = \int d\,\zeta\,x\,(\zeta) = S\,x. \tag{22}$$

Further the time reversal invariance of the equations of motion (11) is expressed by the commutation relation

$$T\,U\,(t) = U\,(-t)\,T. \tag{23}$$

If in particular we apply the time reversal operator T to the phase functions a (4) which correspond to the macroscopic observables A (3) we obtain n phase functions

$$T\,a = (T\,a^1,\ \dots,\ T\,a^n) \tag{24}$$

which may be said to correspond to the macroscopic observables

$$T\,A = (T\,A^1,\ \dots,\ T\,A^n). \tag{25}$$

In (6) we defined the indicator function $I\,(i)$ corresponding to values of the n-dimensional observable A in the interval (5). It is evident that

$$T\,I\,(i) \tag{26}$$

is the indicator function corresponding to values of the time reversed observable $T\,A$ (25) in the interval i.

The structure function corresponding to the experiment discussed above is now defined in analogy to (7)

$$V\,(i_1,\,i_2;\,t_1,\,t_2;\,A) = S\,[U\,(t_1)\,I\,(i_1)]\,[U\,(t_2)\,I\,(i_2)]. \tag{27}$$

From the invariance property (17) it follows directly that the structure function depends only on the time difference so that we may write

$$V\,(i_1,\,i_2;\,t_1,\,t_2;\,A) = V_2\,(i_1,\,i_2;\,t_2 - t_1;\,A). \tag{28}$$

Further, from the same invariance property

$$V_2(i_1, i_2; t; A) = V_2(i_2, i_1; -t; A),^1 \tag{29}$$

and from the time reversal invariance (22) and the commutation relation (23)

$$V_2(i_1, i_2; t; TA) = V_2(i_2, i_1; t; A). \tag{30}$$

There is no problem in extending the discussion to an arbitrary finite number of measurements of the observable A e.g. at the times

$$t_1 < t_2 < \cdots < t_k. \tag{31}$$

The structure function defined in analogy to (27)

$$V(i_1, \ldots, i_k; t_1, \ldots, t_k; A) = \mathcal{S}\,[U(t_1)\,I(i_1)]\,\ldots\,[U(t_k)\,I(i_k)] \tag{32}$$

will obviously be invariant under a translation of the origin of the time scale

$$V(i_1, \ldots, i_k; t_1 + t, \ldots, t_k + t; A) = V(i_1, \ldots, i_k; t_1, \ldots, t_k; A), \tag{33}$$

and satisfy the time reversal symmetry relation

$$V(i_1, \ldots, i_k; t_1, \ldots, t_k; TA) = V(i_k, \ldots, i_1; t_1, \ldots, t_k; A). \tag{34}$$

The structure functions are connected by the *consistency* relations

$$\begin{aligned} V(i_1, \ldots, i_{k-1}, R^n; t_1, \ldots, t_{k-1}, t_k; A) &= V(i_1, \ldots, i_{k-1}; t_1, \ldots, t_{k-1}; A), \\ V(R^n, i_2, \ldots, i_k; t_1, t_2, \ldots, t_k; A) &= V(i_2, \ldots, i_k; t_2, \ldots, t_k; A) \end{aligned} \tag{35}$$

which follow immediately from the fact that

$$I(R^n) = 1. \tag{36}$$

3.2. *Quantum mechanics*

The equations of motion in the Schrödinger picture generate a one-parameter group of unitary transformations in the state-vector Hilbert space corresponding to the mechanical system

$$u(0)\,\psi = \psi;\ u(t)\,u(t')\,\psi = u(t+t')\,\psi \qquad (-\infty < t,\ t' < +\infty) \tag{37}$$

$$\langle u(t)\,\psi \,|\, u(t)\,\psi\rangle = \langle\psi\,|\,\psi\rangle \ \text{ or } \ u(t)^*\,u(t) = 1. \tag{38}$$

Here ψ is an arbitrary state-vector and $\langle\,|\,\rangle$ denotes the scalar product.

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[1] Symmetries of the type (29) have sometimes been incorrectly interpreted as expressing time reversal symmetry. In reality they are only a reflection of the fact that the equations of motion generate a *group* of *measure preserving* point transformations.

The mechanical system being closed, the equations of motion are invariant under time reversal. Following [Wigner, 1932] we express the time reversal operation as a conjugation operation J in the state-vector space. A conjugation operation is an antilinear, isometric and involutory transformation of the vector space onto itself. That is

$$J\,(\lambda\,\psi + \mu\,\varphi) = \bar{\lambda}\,J\,\psi + \bar{\mu}\,J\,\varphi \qquad \begin{array}{l}(\psi,\ \varphi \text{ arbitrary state-vectors})\\ (\lambda,\ \mu \text{ arbitrary complex numbers})\end{array} \tag{39}$$

$$\langle J\,\psi\,|\,J\,\psi\rangle = \langle\psi\,|\,\psi\rangle \tag{40}$$

$$J^2 = 1. \tag{41}$$

The time reversal invariance of the equations of motion is expressed by

$$J\,u\,(t) = u\,(-t)\,J, \tag{42}$$

or equivalently by the statement that the Hamiltonian is "real", to be understood in the sense that it commutes with the conjugation operator J.

For the purposes of statistical mechanics it is more convenient to use a representation of the kinetic group $u\,(.)$ analogous to Koopman's in classical mechanics, that is to use a Heisenberg picture, and a similar representation of time reversal. Taking $x, y, \ldots$ to be bounded linear operators[1] in the state-vector space we define $U\,(t)$ by

$$U\,(t)\,x = u\,(t)^*\,x\,u\,(t) \qquad (-\infty < t < +\infty). \tag{43}$$

Evidently $U\,(.)$ is a group of isomorphisms of the algebra of all bounded linear operators

$$\begin{aligned} U\,(t)\,[\lambda\,x + \mu\,y] &= \lambda\,U\,(t)\,x + \mu\,U\,(t)\,y \\ U\,(t)\,[x\,y] &= [U\,(t)\,x]\,[U\,(t)\,y] \end{aligned} \tag{44}$$

which commutes with the *-operation, the formation of the Hermitian adjoint

$$[U\,(t)\,x]^* = U\,(t)\,x^*. \tag{45}$$

Further the trace-operation $\mathcal{S}$ is invariant under $U\,(t)$

$$\mathcal{S}\,U\,(t)\,x = \mathcal{S}\,x.^2 \tag{46}$$

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[1] The class of all bounded linear operators on a Hilbert space is a non commutative Banach algebra with a *-operation. The extensive mathematical theory of operator algebras is presented e.g. in [Dixmier, 1957].

[2] The trace of a bounded non negative operator is always defined but possibly equal to $+\infty$. The trace of an arbitrary bounded operator is defined as a sum of four terms corresponding to the decomposition of the operator in non negative parts $x = a - b + i\,c - i\,d$, and has meaning if no expressions of the form $\infty - \infty$ occur in the sum.

We define the time reversal operator T by

$$T\,x=(J\,x\,J)^{*}. \tag{47}$$

From the properties of the conjugation operation J (39), (40), (41) it follows that the time reversal operator T is an involution

$$T\,T=1, \tag{48}$$

an *anti* isomorphism of the algebra of bounded operators

$$\begin{aligned} T\,(\lambda\,x+\mu\,y)&=\lambda\,T\,x+\mu\,T\,y\\ T\,[x\,y]&=[T\,y]\,[T\,x], \end{aligned} \tag{49}$$

which commutes with the *-operation

$$[T\,x]^{*}=T\,x^{*}, \tag{50}$$

and that the trace operation is invariant under T

$$S\,T\,x=S\,x. \tag{51}$$

Further the time reversal invariance (42) of the equations of motion is expressed by

$$T\,u\,(t)=u\,(t), \tag{52}$$

or by

$$T\,U\,(t)=U\,(-t)\,T. \tag{53}$$

Applying in particular the time reversal operator T to the operators a (4) which correspond to the macroscopic observables A (3) we obtain n operators $T\,a$ which correspond to the macroscopic observables $T\,A$.

So far we have profited from the formal structural analogy of the algebra of the bounded functions on the phase space (the algebra of classical observables) and the algebra of the bounded linear operators on the state-vector space (the algebra of quantum mechanical observables).[1] In the definition of the structure function corresponding to the experiment discussed above we must however take into account the non commutativity of the algebra of quantum mechanical observables and the special nature of the quantum mechanical process of measurement.

To begin with, we must consider the decomposition of the unity which corresponds to the oparators a (4) which are associated with the macroscopic observables A (3). This decomposition is given by the projection operators $I\,(.)$

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[1] Most observables are of course represented by unbounded functions or operators, e.g. energy, momentum, angular momentum, but can be associated with bounded functions or operators, e.g. the $I\,(i)$ (6). On the other hand, it is not necessary that every bounded operator corresponds to an observable.

(6) which are defined for each n-dimensional interval. As according to the quantum theory of measurement an observation can distinguish between only finitely many or at most denumerably many elementary events (see e.g. [von Neumann, 1932 a]), we can write

$$I(i) = \sum_{\alpha \in i} I(\alpha), \tag{54}$$

where $I(\alpha)$ denotes the projection operator corresponding to the n-dimensional interval which contains only the point α, and the sum extends over all points α in the interval i. As was stated $I(\alpha) = 0$ except for at most denumerably many points so that the sum in (54) has a well defined meaning.

The structure function corresponding to (27) is now defined by

$$V(i_1, i_2; t_1, t_2; A) = \sum_{\alpha_1 \in i_1} \sum_{\alpha_2 \in i_2} V(\alpha_1, \alpha_2; t_1, t_2; A), \tag{55}$$

where

$$\begin{aligned} V(\alpha_1, \alpha_2; t_1, t_2; A) = \mathcal{S}\,\{[U(t_1)\, I(\alpha_1)]\, [U(t_2)\, I(\alpha_2)]\}^* \times \\ \times \{[U(t_1)\, I(\alpha_1)]\, [U(t_2)\, I(\alpha_2)]\}. \end{aligned} \tag{56}$$

From the invariance property (46) of the trace operation $\mathcal{S}$ it follows as in the corresponding classical case that the structure function depends only on the time difference so that we may write

$$V(i_1, i_2; t_1, t_2; A) = V_2(i_1, i_2; t_2 - t_1; A). \tag{57}$$

From the same invariance property and the relation

$$\mathcal{S}(xy) = \mathcal{S}(yx) \quad (x, y \text{ arbitrary operators in the state-vector space}) \tag{58}$$

we obtain

$$V_2(i_1, i_2; t; A) = V_2(i_2, i_1; -t; A).^1 \tag{59}$$

I follows further, from the time reversal invariance (51) and the commutation relation (53), that

$$V_2(i_1, i_2; t; TA) = V_2(i_2, i_1; t; A). \tag{60}$$

As in the classical case there is no problem in extending the discussion to an arbitrary finite number of measurements of the observables A. The structure function corresponding to measurements at the times (31) is defined in analogy to (55);

$$V(i_1, \ldots, i_k; t_1, \ldots, t_k; A) = \sum_{\alpha_1 \in i_1} \cdots \sum_{\alpha_k \in i_k} V(\alpha_1, \ldots, \alpha_k; t_1, \ldots, t_k; A), \tag{61}$$

where

$$\begin{aligned} V(\alpha_1, \ldots, \alpha_k; t_1, \ldots, t_k; A) = \mathcal{S}\,\{[U(t_1)\, I(\alpha_1)] \ldots [U(t_k)\, I(\alpha_k)]\}^* \times \\ \times \{[U(t_1)\, I(\alpha_1)] \ldots [U(t_k)\, I(\alpha_k)]\}. \end{aligned} \tag{62}$$

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[1] See the note to equation (29), and [Groenwold, 1957].

The structure function (61) will obviously be invariant under a translation of the origin of the time

$$V(i_1, \dots, i_k; t_1+t, \dots, t_k+t; A) = V(i_1, \dots, i_k; t_1, \dots, t_k; A) \qquad (63)$$

and satisfy the time reversal symmetry relation

$$V(i_1, \dots, i_k; t_1, \dots, t_k; TA) = V(i_k, \dots, i_1; t_1, \dots, t_k; A). \qquad (64)$$

The structure functions are connected by the *consistency* relation

$$\begin{aligned} V(i_1, \dots, i_{k-1}, R^n; t_1, \dots, t_{k-1}, t_k; A) &= V(i_1, \dots, i_{k-1}; t_1, \dots, t_{k-1}; A), \\ V(R^n, i_2, \dots, i_k; t_1, t_2, \dots, t_k; A) &= V(i_2, \dots, i_k; t_2, \dots, t_k; A). \end{aligned} \qquad (65)$$

In particular we obtain by "contraction" of V_2 the structure function (7)

$$V_2(i_1, R^n; t; A) = V_2(R^n, i_1; t; A) = V(i_1; A). \qquad (66)$$

The consistency relations (65) and (66) follow directly from the fact that

$$\sum_{\alpha \in R^n} I(\alpha) = I \qquad (67)$$

is the unit operator in the state-vector space.

3.3. *The structure functions corresponding to macroscopic observations*

The structure functions

$$V(i_1, \dots, i_k; t_1, \dots, t_k; A) \qquad (68)$$

defined in the classical case by (32) and in the quantum theoretical case by (61), (62) are according to their definitions non negative, additive set functions in the $(k \cdot n)$-dimensional Euclidean space, and hence define a measure in that space, the "natural measure" in the "phase space of the experiment". It follows from the consistency relations (35), (65) that

$$V(i_1, \dots, i_l, \dots, i_k; t_1, \dots, t_l, \dots, t_k; A) \leq V(i_l; A). \qquad (69)$$

Evidently the "natural measure" of the whole phase space of the experiment will be infinite if the classical phase space has infinite Liouville measure or if the state-vector space is of infinite dimensionality.

The fundamental properties of the structure functions (68) are the consistency relations (35), (65), the stationarity, that is the invariance under translation of the origin of the time, (33), (63), and the time reversal symmetry, (34), (64).

Whereas structure functions derived from the classical theory satisfy the "contraction relation"

$$V(i_1, \ldots, i_{l-1}, R^n, i_{l+1}, \ldots, i_k; t_1, \ldots, t_{l-1}, t_l, t_{l+1}, \ldots, t_k; A) \\ = V(i_1, \ldots, i_{l-1}, i_{l+1}, \ldots, i_k; t_1, \ldots, t_{l-1}, t_{l+1}, \ldots, t_k; A), \tag{70}$$

this is in general not the case for structure functions derived from quantum theory, unless the "contraction relation" (70) reduces to the particular case of a consistency relation. This failure is obviously a reflection of the irreversible character of the (ideal) quantum measurement, that is it is a logical consequence of the fact that gain of information is always connected with a certain loss of information. However, we are here discussing measurements of macroscopic observables and it is intuitively clear that for such observables the irreversible nature of the (ideal) measurement must be completely negligible as otherwise the values of the macroscopic observables could not be used as objective characteristics of macroscopic systems, and hence there would exist nothing such as macroscopic observables and as a consequence no macroscopic systems. As we have no reason to expect that quantum theory is incompatible with macroscopic physics we must assume that the "contraction relation" (70) is approximately valid also for structure functions derived from quantum theory. This gives us a necessary connection between the operators a corresponding to the macroscopic observables A and the Hamiltonian H of the mechanical system, the operators a must "almost"[1] commute with H. Though this statement has an intuitive significance it is not easily formulated quantitatively.

A quantitative measure of the commutativity of the operators a with H can be obtained from a comparison of the density operators

$$\exp\{Y(\beta) - \beta H\} \tag{71}$$

and

$$\sum_{\alpha \in R^n} I(\alpha) \exp\{Y(\beta) - \beta H\} I(\alpha), \tag{72}$$

the first characterizing a canonical ensemble with temperature $(\beta \varkappa)^{-1}$, where $\varkappa$ is Boltzmann's constant, and the second characterizing the same ensemble after the observation of A, without record of the result of the observation. It follows from Klein's lemma, [Klein, 1931] that the entropy corresponding to the second density operator is greater than the entropy corresponding to the first one, and that the entropies are equal if and only if the density operators are equal, that is if and only if the Hamiltonian H is compatible with all the projections $I(\alpha)$. If the operators a shall correspond to macroscopic observables it is therefore necessary but certainly not sufficient that the difference between the two entropies is an unobservable fraction of the total entropy. Even if this condition is physically meaningful it seems difficult to use it as an analytic characterization of operators corresponding to macroscopic observables. There is no difficulty in showing that the condition is fulfilled asymptotically for systems consisting of a large number of similar and independent parts if the operators a are sum-functions.

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[1] An attempt to characterize operators, whose commutator with the Hamiltonian is "small" can be found in [van Kampen, 1956]. Here the emphasize is on the fact that the macroscopic observables are approximate constants of motion.

4. The phase space of an infinite series of observations

We shall consider an idealized experiment which consists in the "continuous" measurement of the observables A (3). By this we mean that the observables are measured at constant, "short" intervals of time

$$\ldots, t, t+t_0, t+2t_0, \ldots, t+kt_0, \ldots \tag{73}$$

and that the series of measurements is infinite in both directions of the time axis. The last assumption is convenient for the mathematical description and is physically irrelevant. Using the time interval between two successive measurements, t_0, as unit we associate each observation with an integer k. The outcome of an experiment is thus an infinite series of points in the n-dimensional Euclidean space:

$$\ldots, \alpha_{-1}, \alpha_0, \alpha_1, \ldots, \alpha_k, \ldots . \tag{74}$$

The totality of possible series of the type (74) will be called the phase space Ω of the experiment, and each possible outcome a phase point ω. The value α_k is the k:th coordinate of the phase point ω.

The class of all finite dimensional structure functions

$$V(i_l, i_{l+1}, \ldots, i_{l+k}; l, l+1, \ldots, l+k; A) \tag{75}$$

satisfying the consistency relations (35) (65), induces a measure $\mu(.)$ in the phase space Ω. The procedure is the same as in the theory of stochastic processes, see e.g. [Kolmogorov, 1933], except for minor changes dependent on the fact that the measure defined by the structure functions is not normalizable. We shall not give the details but only remark that the procedure starts with the construction of the class $\mathfrak{F}$ of so called measurable subsets of Ω. These measurable subsets are generated by all subsets of Ω of the type

$$\{\omega \mid \omega_l \in i_l, \omega_{l+1} \in i_{l+1}, \ldots, \omega_{l+k} \in i_{l+k}\}. \tag{76}$$

The μ-measure assigned to the set (76) is

$$\mu\{\omega \mid \omega_l \in i_l, \ldots, \omega_{l+k} \in i_{l+k}\} = V(i_l, \ldots, i_{l+k}; l, \ldots, l+k; A). \tag{77}$$

Let a point transformation u be defined on Ω by

$$(u\,\omega)_k = \omega_{k+1}. \tag{78}$$

It follows directly from the stationarity of the structure functions (33), (63), that the transformation u preserves the μ-measure in Ω. That is, if F is a set belonging to the class $\mathfrak{F}$, its inverse image, $u^{-1}F$, consisting of all points ω such that $u\,\omega \in F$, belongs to $\mathfrak{F}$ and has the same μ-measure

$$\mu\,(u^{-1}\,F) = \mu\,(F). \tag{79}$$

Evidently the point transformation u describes the kinetics of the experiment discussed above. We have thus obtained a phase space representation of the experiment which is completely analogous to the phase space representation of a mechanical system in the classical theory. However, the phase space representation of the experiment applies both to a classical and to a quantal description of the mechanical system. In both cases the equations of motion generate an incompressible stationary flow in the phase space, determined by the measure preserving point transformation u. Hence it is possible to apply the wellknown methods of classical statistical mechanics: ergodic theory etc. to series of observations in systems, independent of the kind of mechanics by which the systems are described. It should be noted that in the classical case the replacement of the phase space of the system by the phase space of the experiment is not a complication of the description. For obviously the description in terms of the phase space of the experiment is in general much coarser than the original in terms of the phase space of the system, the first description beeing dependent only on the macroscopic observables A. It must be noticed that we have evaded here the fundamental and very difficult problem of actual derivation of the structure functions from classical mechanics or from quantum mechanics respectively.

We shall make the further assumption about the macroscopic observables A (3), that each has a definite parity with respect to time reversal, that is

$$T\,A^{\mu} = \theta\,(\mu)\,A^{\mu},\ \ (\theta\,(\mu) = +1 \ \text{or} \ -1,\ \mu = 1,\ \ldots,\ n). \tag{80}$$

With this assumption the time reversal symmetry of the structure functions (34) (64) can be expressed as

$$\begin{aligned} V\,(\theta\,i_1,\ \ldots,\ \theta\,i_k;\ t_1,\ \ldots,\ t_k;\ A) &= V\,(i_k,\ \ldots,\ i_1;\ t_1,\ \ldots,\ t_k;\ A) \\ &= V\,(i_1,\ \ldots,\ i_k;\ -t_k,\ \ldots,\ -t_1;\ A) \end{aligned} \tag{81}$$

where $\theta\,i$ is the "time reversed" n-dimensional interval

$$\alpha \in \theta\,i \ \text{if} \ \theta\,\alpha = (\theta\,(1)\,\alpha^1,\ \ldots,\ \theta\,(n)\,\alpha^n) \in i. \tag{82}$$

We define the point transformation τ in Ω by

$$(\tau\,\omega)_{-k} = \theta\,\omega_k = (\theta\,(1)\,\omega_k^1,\ \ldots,\ \theta\,(n)\,\omega_k^n) \tag{83}$$

and find directly that τ is involutory, and from (81) that τ preserves the measure $\mu\,(.)$. Further τ is connected with the kinetic transformation u by

$$\tau\,u = u^{-1}\,\tau. \tag{84}$$

5. The incompressible flow in the phase space

For the description of series of observations in a mechanical system we have developed the structure

$$\Omega,\ \mathfrak{F},\ \mu(.),\ u,\ \tau, \tag{85}$$

consisting of a phase space Ω with a class of measurable subsets $\mathfrak{F}$ and a measure $\mu(.)$, in general with $\mu(\Omega)=\infty$, a measure preserving point transformation u, generating an incompressible flow in Ω, and finally a measure preserving, involutory transformation τ connected with u by the relation (84) which expresses the invariance of the fundamental equations of motion under time reversal. That is we have a structure formally analogous to classical mechanics. In this section we shall discuss some questions related to the flow in Ω generated by u, in particular the classical problem of recurrences.

It was recognized already by the founders of statistical mechanics, in particular by Boltzmann and by Gibbs, that the physically relevant constituents of the classical phase space are not the individual phase points but those subsets of the phase space which have a positive Liouville-measure, though the physical reasons could be properly understood only after the discovery of the quantum theory, and though a logically consistent formulation was possible only after the invention of the mathematical measure theory by Lebesgue.[1] The measurable subsets (the so called Borel sets) of the phase space may be said to form the class of possible *events* with reference to *all possible* observations of the system. Two events differing from each other by a set (an event) of Liouville-measure zero are physically equivalent. However, a macroscopic observer can realize not all possible events but only a certain subclass, even if he can repeat his experiment an arbitrary number of times. We shall call this "coarser" subclass of all possible events the *observable events*. It is clear from our previous analysis that the observable events of the experiment considered above constitute exactly the class $\mathfrak{F}$ of measurable subsets of the phase space Ω of the experiment.

The transition time

If Δ is an arbitrary subset of the phase space Ω, belonging to the class $\mathfrak{F}$ we consider a phase point which enters[2] the set at the time $t=1$, and then remains in Δ until the time $t=k+1$. We shall say that the transition time of the particular phase point is equal to k. We want to characterize the set Δ relative to the flow in the phase space generated by the point transformation u. This could be done for instance by associating each possible transition time with a probability. For the computation of these probabilities we shall mainly use some ideas due to Kac [Kac, 1959]. For the first considerations it is not essential that the flow generated by u is incompressible and that u is invertible.

A point $\omega \in \Omega$ has the transition time k exactly if[3]

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[1] As regards Boltzmann's point of view see [Ehrenfest, 1911], in particular note 170. The second proof of the recurrence theorem, given by Gibbs [Gibbs, 1902] in particular, anticipates measure theoretical methods and is free from the irrelevant topological considerations of the original proofs due to Poincaré and Zermelo.

[2] I apologize for using the word point in a double sense.

[3] The set $\complement\,\Delta$ is the complement, "not Δ", of Δ in Ω.

$$\begin{array}{lll}
\omega \in \complement\,\Delta & \text{or equivalently} & \omega \in \complement\,\Delta \\
u\,\omega \in \Delta & \quad ,, \qquad ,, & \omega \in u^{-1}\,\Delta \\
\cdots & \cdots & \cdots \\
u^{k}\,\omega \in \Delta & \text{or equivalently} & \omega \in u^{-k}\,\Delta \\
u^{k+1}\,\omega \in \complement\,\Delta & \quad ,, \qquad ,, & \omega \in u^{-(k+1)}\,\complement\,\Delta .
\end{array} \tag{86}$$

The set (belonging to $\mathfrak{F}$) of all points which enter Δ at $t = 1$ and leave Δ for the first time at $t = k + 1$ is thus simply the intersection of the sets occurring at the right hand side in (86)

$$\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta.^{1} \tag{87}$$

We shall assume that

$$0 < \mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} < \infty. \tag{88}$$

The "probability" $p(k)$ for a transition time equal to k is defined by

$$p(k)\,\mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} = \mu\{\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\}, \tag{89}$$

that is, $p(k)$ is the ratio of the measure of the set of all points entering Δ at $t = 1$ and leaving Δ at $t = k + 1$ for the first time to the measure of the set of all points entering Δ at $t = 1$. It is evident that

$$\begin{aligned}
&\mu\{\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\} \\
&\qquad = \mu\{\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta\} - \mu\{\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-(k+1)}\,\Delta\},
\end{aligned} \tag{90}$$

and that the sets

$$\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \tag{91}$$

decrease monotonically with k to

$$\complement\,\Delta \bigcap_{\nu=1}^{\nu=\infty} u^{-\nu}\,\Delta, \tag{92}$$

that is the set of all points entering Δ at $t = 1$ and remaining for ever in Δ. Hence we find

$$\begin{aligned}
\sum_{k=1}^{k=\infty} p(k)\,\mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} &= \mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} - \mu\{\complement\,\Delta \bigcap_{\nu=1}^{\nu=\infty} u^{-\nu}\,\Delta\} \leqslant \\
&\leqslant \mu\{\complement\,\Delta \cap u^{-1}\,\Delta\}
\end{aligned} \tag{93}$$

or

$$\sum_{k=1}^{k=\infty} p(k) = 1 - p(\infty) \leqslant 1, \tag{94}$$

---

[1] $\Delta_1 \cap \Delta_2$ denotes the intersection of the two sets Δ_1 and Δ_2, that is the set of all points which are contained in both of the sets.

where $p(\infty)$ is the probability of an "infinite transition time"

$$p(\infty)\,\mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} = \mu\{\complement\,\Delta \bigcap_{\nu=1}^{\nu\;\infty} u^{-\nu}\,\Delta\}, \tag{95}$$

that is the "probability" that a particle enterning Δ at $t = 1$ will remain in Δ for ever.

Consider now a point which is in Δ at the time $t = 0$ and moves on in Δ exactly until the time $t = k$. A point ω remains in Δ, k units of time precisely when

$$\begin{array}{lll} \omega \in \Delta & \text{or equivalently} & \omega \in \Delta \\ u\,\omega \in \Delta & \text{,,} \qquad\qquad \text{,,} & \omega \in u^{-1}\,\Delta \\ \cdots & \cdots & \cdots \\ u^{k-1}\,\omega \in \Delta & \text{or equivalently} & \omega \in u^{-(k-1)}\,\Delta \\ u^{k}\,\omega \in \complement\,\Delta & \text{,,} \qquad\qquad \text{,,} & \omega \in u^{-k}\,\complement\,\Delta. \end{array} \tag{96}$$

The set (belonging to $\mathfrak{F}$) of all points in Δ which remain in Δ k units of time is the intersection of the sets occurring at the right hand side of (96)

$$\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-(k-1)}\,\Delta \cap u^{-k}\,\complement\,\Delta. \tag{97}$$

In addition to (88) we shall assume that

$$0 < \mu(\Delta) < \infty. \tag{98}$$

The "probability" $q(k)$ that a point in Δ will remain in Δ exactly k units of time is defined by

$$q(k)\,\mu(\Delta) = \mu(\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-(k-1)}\,\Delta \cap u^{-k}\,\complement\,\Delta), \tag{99}$$

that is $q(k)$ is the ratio of the measure of the set of all points in Δ at $t = 0$ which leave Δ at $t = k$ for the first time, to the measure of the set of all points in Δ at $t = 0$. Evidentally

$$\begin{aligned} &\mu\{\Delta \cap u^{-1}\Delta \cap \cdots \cap u^{-(k-1)}\,\Delta \cap u^{-k}\,\complement\,\Delta\} \\ &\qquad = \mu\{\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-(k-1)}\,\Delta\} - \mu\{\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta\}, \end{aligned} \tag{100}$$

and the sets

$$\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \tag{101}$$

decrease monotonically with k to

$$\bigcap_{\nu=0}^{\nu=\infty} u^{-\nu}\,\Delta, \tag{102}$$

that is the set of all points in Δ at $t = 0$ which remain for ever in Δ. Hence we find

$$\sum_{k=1}^{k=\infty} q(k)\,\mu\{\Delta\} = \mu\{\Delta\} - \mu\{\bigcap_{\nu=0}^{\nu=\infty} u^{-\nu}\,\Delta\} \leqslant \mu\{\Delta\} \tag{103}$$

or

$$\sum_{k=1}^{k=\infty} q(k) = 1 - q(\infty) \leqslant 1, \tag{104}$$

where $q(\infty)$ is the probability that a point in Δ leaves Δ "after an infinite time", that is remains for ever in Δ

$$q(\infty)\,\mu\{\Delta\} = \mu\{\bigcap_{\nu=0}^{\nu=\infty} u^{-\nu}\,\Delta\}. \tag{105}$$

We shall now see how the "probabilities" $p(.)$ and $q(.)$ are related. Here for the first time we make explicit use of the measure preserving property of u:

$$\mu\{u^{-1}\,\Delta'\} = \mu\{\Delta'\} \qquad (\text{arbitrary } \Delta' \in \mathfrak{F}). \tag{106}$$

It follows directly that

$$\begin{aligned} &\mu\{\complement\,\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\} \\ &\qquad = \mu\{u^{-1}\,\Delta \cap u^{-2}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\} - \\ &\qquad\qquad - \mu\{\Delta \cap u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\}, \end{aligned} \tag{107}$$

and it follows from the condition (106) that

$$\mu\{u^{-1}\,\Delta \cap \cdots \cap u^{-k}\,\Delta \cap u^{-(k+1)}\,\complement\,\Delta\} = \mu\{\Delta \cap \cdots \cap u^{-(k-1)}\,\Delta \cap u^{-k}\,\complement\,\Delta\}. \tag{108}$$

Combining (107), (108) and the definitions (89) and (99) we find the desired connection between $p(.)$ and $q(.)$

$$p(k)\,\mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} = [q(k) - q(k+1)]\,\mu\{\Delta\}. \tag{109}$$

We introduce the generating functions

$$P(z) = \sum_{k=0}^{k=\infty} p(k)\,e^{-kz} \qquad (z \geqslant 0), \tag{110}$$

and

$$Q(z) = \sum_{k=0}^{k=\infty} q(k)\,e^{-kz} \qquad (z \geqslant 0), \tag{111}$$

which are welldefined according to (94) and (104). From (109) follows the relation between the generating functions

$$P(z)\,\mu\{\complement\,\Delta \cap u^{-1}\,\Delta\} = [Q(z)\,(1 - e^{z})]\,\mu\{\Delta\} + \mu\{\Delta \cap u^{-1}\,\complement\,\Delta\}. \tag{112}$$

Using (106) we find

$$\mu\{\complement\Delta \cap u^{-1}\Delta\} = \mu\{\Delta \cap u^{-1}\complement\Delta\} = q(1)\,\mu(\Delta), \tag{113}$$

expressing the ballance of "incompressible fluid": the measure of the sets of points entering Δ in the unit of time is equal to the measure of the sets of points leaving Δ in the unit of time.

Hence we can write (112) as

$$P(z)\,q(1) = Q(z)\,[1-e^{z}] - q(1). \tag{114}$$

The limit for $z \downarrow 0$ of (114) exists as a consequence of (104)

$$P(0)\,q(1) = Q(0)\cdot 0 + q(1) = q(1), \tag{115}$$

and as in view of the assumption (88) $q(1) > 0$, we find

$$P(0) = \sum_{k=1}^{k=\infty} p(k) = 1 \text{ or equivalently } p(\infty) = 0. \tag{116}$$

The trivial meaning of this being that, the flow being incompressible, almost every point entering Δ will leave Δ after a finite time. We now find the derivative of $P(z)$ at $z=0$.

$$P'(0) = \lim_{z\downarrow 0} \frac{P(z)-1}{z} = \lim_{z\downarrow 0} \frac{Q(z)}{q(1)}\,\frac{1-e^{z}}{z} = -\frac{Q(0)}{q(1)}, \tag{117}$$

or using the definitions of $P(z)$ and $Q(z)$, (110) and (111),

$$t_{\text{trans}}(\Delta) = \sum_{k=1}^{k=\infty} p(k)\,k = \frac{Q(0)}{q(1)} = \frac{1-q(\infty)}{q(1)}, \tag{118}$$

that is the *mean transition time* $t_{\text{trans}}(\Delta)$ for the set Δ is equal to the "probability" that an arbitrary point in Δ does not remain for ever in Δ, divided by the "probability" that the point leaves Δ in the unit of time.[1]

We recall the formal definition (105) of $q(\infty)$ in terms of the measure of the set

$$\bigcap_{\nu=0}^{\nu=\infty} u^{-\nu}\Delta \tag{119}$$

contained in Δ. The sets

$$\bigcap_{\nu=\mu}^{\nu=\infty} u^{-\nu}\Delta = u^{-\mu}\Big\{\bigcap_{\nu=0}^{\nu=\infty} u^{-\nu}\Delta\Big\} \tag{120}$$

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[1] An alternative derivation of this result is given in the appendix.

form an increasing sequence and have all the same measure as (119). Define

$$\Delta_* = \bigcup_{\mu=0}^{\mu=\infty} \bigcap_{\nu=\mu}^{\nu=\infty} u^{-\nu}\Delta. \tag{121}$$ [1]

It follows from the construction that Δ_* is u-invariant

$$u^{-1}\Delta_* = \Delta_* \tag{122}$$

and contains the set (119). On the other hand the two sets have the same measure and are hence equivalent. If and only if Δ contains no subset which is equivalent to a u-invariant set, we have according to (105)

$$q(\infty) = 0 \text{ or equivalently } \mu(\Delta_*) = 0. \tag{123}$$

If (123) holds we shall say that the set Δ is transitory. Hence we have for a transitory set the mean transition time

$$t_{\text{trans}}(\Delta) = \frac{1}{q(1)} = \frac{\mu(\Delta)}{\mu(\Delta \cap u^{-1} \complement \Delta)} \tag{124}$$

and for an arbitrary set

$$t_{\text{trans}}(\Delta) = \frac{\mu(\Delta \cap \complement \Delta_*)}{\mu(\Delta \cap u^{-1} \complement \Delta)} \tag{125}$$

Unfortunately the relation (113) cannot be used in general to derive the dispersion of the transition time.

The recurrence time

By the mean recurrence time of the set Δ one would understand the mean transition time of the complementary set. To obtain a proper definition we consider the set

$$\bigcup_{\nu=0}^{\nu=\infty} u^{-\nu}\Delta \tag{126}$$

of all points of Ω which reach Δ at some finite time. We assume that the μ-measure of this set is finite. Hence the u-invariant set

$$\Delta^* = \bigcap_{\mu=0}^{\mu=\infty} \bigcup_{\nu=\mu}^{\nu=\infty} u^{-\nu}\Delta \tag{127}$$

has the same finite μ-measure and is equivalent to (126). Up to equivalence relative to sets of μ-measure zero we have then,

$$\Delta_* \subset \Delta \subset \Delta^* \tag{128}$$

---

[1] $\bigcup_{\nu} F_\nu$ denotes the union of the sets F_ν, that is the set of all points contained in one at least of the sets F_ν.

that is the set Δ is contained in the u-invariant set Δ^*, of finite measure, and Δ^* is the "smallest" u-invariant set containing Δ, whereas Δ_* (121) is the "greatest" u-invariant set contained in Δ. The mean recurrence time of the set Δ is defined as the mean transition time of the complement of Δ in Δ^*, that is of $\Delta^* \cap \complement \Delta$. Hence according to (118)

$$t_{\text{rec}}(\Delta) = t_{\text{trans}}(\Delta^* \cap \complement \Delta) = \frac{1 - q_c(\infty)}{q_c(1)}. \tag{129}$$

It is easily seen that

$$q_c(1) = q(1) \frac{\mu(\Delta)}{\mu(\Delta^*) - \mu(\Delta)}. \tag{130}$$

The relation (116) applied to $p_c(.)$ is an expression of Poincaré's recurrence theorem: any point of Δ recurs in a finite time if Δ is contained in a invariant set of finite measure. If in particular the complement of Δ in Δ^* is transitory (123) we have $q_c(\infty) = 0$ and the mean recurrence time is

$$t_{\text{rec}} = \frac{\mu(\Delta^*) - \mu(\Delta)}{q(1)\, \mu(\Delta)}. \tag{131}$$

We note that (131) is true whether Δ itself is transitory or not.

In the conventional terminology the transformation u is called metrically transitive or ergodic if it has only trivial invariant sets, that is if

$$u^{-1} \Delta' = \Delta' \text{ implies } \mu(\Delta') = 0 \text{ or } \mu(\complement \Delta') = 0. \tag{132}$$

In this case every set of positive finite measure is transitory. However, in the particular structure (85) corresponding to the observation of macroscopic observables the transformation u will hardly ever be ergodic.

Regenerative sets

In (106) the condition of incompressibility was introduced, and the subsequent discussion was based on this condition. However it is of some interest to replace this condition by the following. The set Δ will be called regenerative[1] if (88) and (98) are satisfied and if

$$p(k) = q(k) \qquad (k = 1, 2, \ldots), \tag{133}$$

$$\mu\{u^{-1} \Delta \cap u^{-2} \Delta \cap \ldots \cap u^{-k} \Delta \cap u^{-(k+1)} \complement \Delta\} = p(k)\, \mu\{u^{-1} \Delta\}, \quad (k = 1, 2, \ldots). \tag{134}$$

The meaning of (133) is that for a point the "probability" of leaving the set Δ in k steps is independent of the past of the point, and (134) expresses a weaker form of incompressibility, the stationarity of the probality distribution of the transition times. We now replace (107) by the assumption that the set Δ is regenerative. The relation (107) holds also under the condition (134) and gives rise to

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[1] The notation is chosen in analogy to the concept regenerative process, see [Feller, 1950].

$$p(k)\,\mu\{\complement\Delta \cap u^{-1}\Delta\} = p(k)\,\mu\{u^{-1}\Delta\} - p(k+1)\,\mu\{\Delta\}. \tag{135}$$

Defining the generating function $P(z)$ by (110) we get from (135) after an elementary calculation

$$P(z) = \frac{p(1)}{e^{z} - 1 + p(1)} \quad \text{or} \quad p(k) = p(1)\,[1 - p(1)]^{k-1}, \tag{136}$$

and the whole probability distribution $p(\,.\,)$ is determined by $p(1)$. In particular we find

$$P(0) = \sum_{k=1}^{k=\infty} p(k) = 1, \qquad \text{or equivalently } p(\infty) = q(\infty) = 0, \tag{137}$$

$$-P'(0) = \sum_{k=1}^{k=\infty} p(k)\,k = \frac{1}{p(1)} = t_{\text{trans}}(\Delta), \tag{138}$$

and for the variance of the transition time

$$\sum_{k=1}^{k=\infty} p(k)\,[k - t_{\text{trans}}(\Delta)]^2 = P''(0) - [P'(0)]^2 = \frac{1 - p(1)}{p(1)^2} = t_{\text{trans}}(\Delta)\,[t_{\text{trans}}(\Delta) - 1]. \tag{139}$$

Hence the expression for the mean transition time is the same as (124) corresponding to the condition (107) and a transitory set. It is obviously possible to combine the conditions (107) and (133), (134). It must however be observed that the expression (139) for the variance is valid in general only if the set Δ is regenerative. Further it must be noticed that the fact that Δ is regenerative does not imply that the complementary set is regenerative. Hence the distribution of the recurrence time cannot be obtained in a simple way.

Variance of the transition time

We consider a set Δ with the mean transition time $t_{\text{trans}}(\Delta)$ given by (118), (125). In general the transition time will vary considerably among the points which enter Δ. That means that points entering Δ simultaneously will leave Δ at very different times and a certain stirring of the phase points in Δ (in Gibbs' sense) occurs. The variance of the transition time is a measure of the stirring produced by the transformation u in the set Δ. If this variance is finite it may be formally obtained from the generating function $P(z)$ (114)

$$\sum_{k=1}^{k=\infty} p(k)\,[k - t_{\text{trans}}(\Delta)]^2 = \frac{2\sum q(k)\,k}{q(1)} - t_{\text{trans}}(\Delta)\,[t_{\text{trans}}(\Delta) + 1], \tag{140}$$

but this expression is in general of no practical use as we cannot estimate the value of $\sum_{k=1}^{k=\infty} q(k)k$. Intuitively looking at the physical interpretation one would be inclined to assume that

$$\sum_{k=1}^{\infty} q(k)\,k \leqslant t_{\text{trans}}(\Delta) \tag{141}$$

and this holds for "tubes of flow" (see appendix), but cannot be proved for arbitrary sets.

Product flow

If the mechanical system which we are considering consists of two (dynamically) independent parts the phase space structure (85) will be the direct product of two structures

$$\Omega_i,\ \mathfrak{F}_i,\ \mu_i(\,.\,),\ u_i,\ \tau_i, \qquad (i=1,2), \tag{142}$$

in the sense that each phase point in Ω is represented by a pair of phase points, one in Ω_1 and one in Ω_2

$$\omega=(\omega_1,\omega_2), \tag{143}$$

the invariant measure $\mu(\,.\,)$ in Ω is the product measure

$$\mu(\Delta_1\times\Delta_2)=\mu_1(\Delta_1)\,\mu_2(\Delta_2);\ \ \Delta_1\in\mathfrak{F}_1,\ \Delta_2\in\mathfrak{F}_2, \tag{144}$$

and the transformations u and τ are given by

$$u\,\omega=(u_1\,\omega_1,\ u_2\,\omega_2), \tag{145}$$

$$\tau\,\omega=(\tau_1\,\omega_1,\ \tau_2\,\omega_2). \tag{146}$$

We shall determine the mean transition time and the mean recurrence time for a product set $\Delta=\Delta_1\times\Delta_2$. We shall first consider $q(1)$, (99), the "probability" that an arbitrary point in the set will leave the set in the unit of time. By definition

$$q(1)=\frac{\mu\{\Delta\cap u^{-1}\complement\Delta\}}{\mu\{\Delta\}} \tag{147}$$

and the definitions of $q_1(1)$ and $q_2(1)$ are analogous. It is easily found by a formal calculation that

$$q(1)=q_1(1)+q_2(1)-q_1(1)\,q_2(1), \tag{148}$$

but a direct probabilistic reasoning is simpler: A point $\omega=(\omega_1,\omega_2)$ in $\Delta=\Delta_1\times\Delta_2$ remains in Δ in the first unit of time exactly if ω_1 remains in Δ_1 and ω_2 remains in Δ_2. These events are independent and it follows that the probability of the combined event is $1-q=(1-q_1)(1-q_2)$. This is exactly (148). Hence we find the mean transition time

$$t_{\text{trans}}(\Delta_1\times\Delta_2)=\frac{1-q(\infty)}{q_1(1)+q_2(1)-q_1(1)\,q_2(1)} \tag{149}$$

and the mean recurrence time, see (129),

$$t_{\mathrm{rec}}(\Delta_1 \times \Delta_2) = \frac{1 - q_c(\infty)}{q_1(1) + q_2(1) - q_1(1)\, q_2(1)} \; \frac{\mu_1(\Delta_1^*)\, \mu_2(\Delta_2^*) - \mu_1(\Delta_1)\, \mu_2(\Delta_2)}{\mu_1(\Delta_1)\, \mu_2(\Delta_2)}. \tag{150}$$

The result can be extended without difficulty to the product of an arbitrary number of phase spaces, that is to systems consisting of an arbitrary number of independent parts. We recall that the time interval t_0 between successive observations was chosen as the unit of time. Hence the mean transition time is in arbitrary units equal to $t_0 \cdot t_{\mathrm{trans}}(\Delta)$. Assuming $q_1(1)$ and $q_2(1)$ to be of the order of t_0

$$q_i(1) = \gamma_i t_0 + o(t_0); \qquad (i = 1, 2), \tag{151}$$

we can replace (148) by

$$\gamma = \gamma_1 + \gamma_2 + o(1) \tag{152}$$

and for an arbitrary number N of "components"

$$\gamma = \sum_{\nu=1}^{\nu=N} \gamma_\nu + o(1) = N \bar{\gamma} + o(1). \tag{153}$$

With the notation

$$\bar{\mu}^N = \prod_{\nu=1}^{\nu=N} \frac{\mu_\nu(\Delta_\nu)}{\mu_\nu(\Delta_\nu^*)}, \tag{154}$$

the mean transition and the mean recurrence times can be expressed by

$$t_{\mathrm{trans}}\left(\prod_{\nu=1}^{\nu=N} \Delta_\nu\right) = \frac{1 - q(\infty)}{N \bar{\gamma}} + o(1), \tag{155}$$

and

$$t_{\mathrm{rec}}\left(\prod_{\nu=1}^{\nu=N} \Delta_\nu\right) = \frac{1 - q_c(\infty)}{N \bar{\gamma}} \; \frac{1 - \bar{\mu}^N}{\bar{\mu}^N} + o(1). \tag{156}$$

Noticing that the geometric mean (154) $\bar{\mu} \leqslant 1$ one obtains from (156) an impression of the behaviour of the mean recurrence time, frequently called the Poincaré cycle $\bar{\mu}$, for a product set of a large number of components corresponding to independent systems, as far as $q_c(\infty)$ can be estimated. For the particular case of recurrences in the angular variables of a system of harmonic oscillators an expression equivalent to (156) has been derived in [Hemmer, Maximon and Wergeland, 1958] by a different method originally developed by Smoluchowski [Smoluchowski, 1916].

Asymptotic distribution of the transition time

The discussion of product flow under the additional assumption (151) could also have ben based directly on the continuous analogue of equation (109). To obtain this analogue we rewrite (109)

$$\frac{q(1)}{t_0}\sum_{k=1}^{k=\frac{t}{t_0}} p(k) = -\frac{1}{t_0}\left[\sum_{k=1}^{k=\frac{t+t_0}{t_0}} q(k) - \sum_{k=1}^{k=\frac{t}{t_0}} q(k)\right] + \frac{q(1)}{t_0} \tag{157}$$

and obtain for fixed t in the limit $t_0 \downarrow 0$

$$\gamma\,[1-\mathcal{D}(t)] = \frac{d}{dt}Q(t) \tag{158}$$

where $\mathcal{D}(t)$ denotes the probability of a transition time shorter than t, and $Q(t)$ denotes the probability that an arbitrary point in the set considered will leave this set before the elapse of the time t, and evidently

$$\gamma = Q'(0). \tag{159}$$

It is easily found that the set Δ is regenerative,

$$\mathcal{D}(t) \equiv Q(t) \qquad \text{exactly if } \mathcal{D}(t) = 1 - e^{-\gamma t}, \tag{160}$$

that is if the transition time is exponentially distributed.

For an arbitrary product flow we have by a simple probabilistic argument

$$1 - Q(t) = [1 - Q_1(t)]\,[1 - Q_2(t)] \tag{161}$$

and a corresponding formula for several components

$$1 - Q(t) = \prod_{\nu=1}^{\nu=N} [1 - Q_\nu(t)]. \tag{162}$$

Consider for simplicity the particular case of equal distributions

$$Q_\nu(t) = Q_1(t) \qquad (\nu = 1, \ldots, N) \;\; Q_1'(0) = \gamma_1. \tag{163}$$

It is then easily found that the transition time divided by the number N of components is asymptotically exponentially distributed for large numbers N. The result follows from the fact that

$$1 - Q\left(\frac{t}{N}\right) = \left[1 - Q_1\left(\frac{t}{N}\right)\right]^N = \left[1 - Q_1'(0)\frac{t}{N} + o\left(\frac{t}{N}\right)\right]^N \rightarrow$$
$$\rightarrow e^{-Q_1'(0)t} = e^{-\gamma_1 t} \qquad (t \text{ fixed, } N \rightarrow \infty). \tag{167}$$

The same asymptotic form of the distribution is obtained also if the $Q_\nu(t)$ are different, if the difference is "not too great". Hence a product set of many components is asymptotically regenerative. We note that the direct product of regenerative sets is again a regenerative set.

In principle it is possible to determine the distribution of the recurrence time of a product set by an analogous method but the combinatorial difficulties are extreme.

Recurrence and macroscopic observables

It will usually be possible to decompose the phase space Ω (85) whose μ-measure is infinite, into a sum of disjoint u-invariant, and not further decomposable subsets of finite μ-measure, each characterized by the numerical value(s) of some macroscopic integral(s). In particular it will often be natural to assume that a measurement (possibly successive measurements) of the macroscopic observables A will determine the macroscopic energy.

Any macroscopic observable associated with the experiment discussed above (section 4) is represented by a function on the phase space which determines the corresponding structure function. For certain types of macroscopic observables in large systems it is possible to obtain an asymptotic expression for the structure function with the aid of the central limit theorem. Let in particular $x(\omega)$ be a function on Ω representing a macroscopic observable, such that the structure function corresponding to the pair

$$x_0(\omega) = x(\omega), \quad x_t(\omega) = x(u^t\omega) \tag{168}$$

is approximately of the Gaussian form

$$V_2(dx, dy; t) = \tag{169}$$

$$= C \frac{1}{2\pi\sigma^2\sqrt{1-\varrho(t)^2}} \exp\left\{\frac{(x-m)^2 + (y-m)^2 - 2\varrho(t)(x-m)(y-m)}{\sigma^2(1-\varrho(t)^2)}\right\} dx\,dy.$$

Here $\varrho(t)$ is the correlation coefficient

$$0 \leqslant \varrho(t) \leqslant 1; \ \lim_{t\to 0} \varrho(t) = 1; \ \varrho(-t) = \varrho(t), \tag{170}$$

and σ^2 is of the order of the number of "independent, similar" components of the system. Note that the parameters C, m and σ^2 are independent of the time. We are interested in the mean recurrence time for a set of the form

$$\{\omega \mid \xi_0 < x(\omega) - m \leqslant \xi\}. \tag{171}$$

We start with the particular case $\xi_0 = -\infty$, and assuming the existence of the limit $\gamma = \lim\limits_{t_0 \downarrow 0} \frac{q(1)}{t_0}$ (151) we have

$$\gamma = \frac{\lim\limits_{t\downarrow 0} \frac{1}{t} \int\limits_{x\leqslant\xi} \int\limits_{y>\xi} \frac{1}{2\pi\sigma^2\sqrt{1-\varrho(t)^2}} \exp\left\{-\frac{x^2+y^2-2\varrho(t)\,xy}{2\sigma^2(1-\varrho(t)^2)}\right\} dx\,dy}{\int\limits_{x\leqslant\xi} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}\frac{x^2}{\sigma^2}\right\} dx}. \tag{172}$$

Introducing the distribution function of the normalized Gaussian distribution

$$\Phi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x}\exp\left\{-\frac{1}{2}y^2\right\}dy, \tag{173}$$

we can rewrite (172) as

$$\gamma=\lim_{t\downarrow 0}\frac{\dfrac{1}{t}\displaystyle\int_{x>\xi}\Phi\left(\frac{\xi-\varrho x}{\sigma\sqrt{1-\varrho^2}}\right)d_x\Phi\left(\frac{x}{\sigma}\right)}{\Phi\left(\dfrac{\xi}{\sigma}\right)} \tag{174}$$

where $\varrho=\varrho(t)$. And it is found that

$$\gamma=\lim_{t\downarrow 0}\frac{\sqrt{1-\varrho}}{t}\,\frac{\dfrac{1}{\sqrt{\pi}}\,\Phi'\left(\dfrac{\xi}{\sigma}\right)}{\Phi\left(\dfrac{\xi}{\sigma}\right)}. \tag{175}$$

To see this we set $z=\dfrac{\xi-\varrho x}{\sigma\sqrt{1-\varrho^2}}$ and obtain

$$\int_{x>\xi}\Phi\left(\frac{\xi-\varrho x}{\sigma\sqrt{1-\varrho^2}}\right)d_x\Phi\left(\frac{x}{\sigma}\right)=\frac{\sqrt{1-\varrho^2}}{\varrho}\int_{-\infty}^{\frac{\xi}{\sigma}\sqrt{\frac{1-\varrho}{1+\varrho}}}\Phi(z)\,\Phi'\left(\frac{\xi-\sigma\sqrt{1-\varrho^2}\,z}{\sigma\varrho}\right)dz. \tag{176}$$

After integration by parts we find that (176) is equal to

$$\sqrt{\frac{1-\varrho}{\pi}}\,\Phi'\left(\frac{\xi}{\sigma}\right)+o\left(\sqrt{1-\varrho}\right), \tag{177}$$

which gives the desired result (175). For a finite interval (ξ_0,ξ) we obtain in the same way

$$\gamma=\lim_{t\downarrow 0}\frac{\sqrt{1-\varrho(t)}}{t}\,\frac{1}{\sqrt{\pi}}\,\frac{\Phi'\left(\dfrac{\xi_0}{\sigma}\right)+\Phi'\left(\dfrac{\xi}{\sigma}\right)}{\Phi\left(\dfrac{\xi}{\sigma}\right)-\Phi\left(\dfrac{\xi_0}{\sigma}\right)}, \tag{178}$$

which includes (175) as a particular case. Assuming the existence of a sufficient number of derivatives, we have

$$\varrho(t)=1+\varrho'(0)\,t+\tfrac{1}{2}\varrho''(0)\,t^2+o(t^2),\qquad \varrho''(0)\leqslant 0, \tag{179}$$

and hence

$$\lim_{t\downarrow 0}\frac{\sqrt{1-\varrho(t)}}{t}=\sqrt{-\frac{1}{2}\varrho''(0)}\quad\text{if }\varrho'(0)=0, \tag{180}$$

otherwise the limit does not exist. That is the derivative of the correlation coefficient must be a function continuous at $t = 0$ (compare (170)). This on the other hand is exactly the necessary and sufficient condition for the existence of the "velocity"

$$\frac{d}{dt} x_t(\omega),$$

which, as is easily seen, has the correlation coefficient $\varrho''(t)$. It is wellknown that many probabilistic models of physical processes violate this condition and are invalid for small times. In particular this is so for models of the Brownian motion type. This fact was strongly emphasized already by Smoluchowski [Smoluchowski, 1916] and again discussed in connection with the linear theory of irreversible processes [Casimir, 1945].

From (178) we readily obtain the mean transition time for the set (171)

$$t_{\text{trans}} = \frac{\Phi\left(\frac{\xi}{\sigma}\right) - \Phi\left(\frac{\xi_0}{\sigma}\right)}{\sqrt{-\frac{\varrho''(0)}{2\pi}}\left[\Phi'\left(\frac{\xi_0}{\sigma}\right) + \Phi'\left(\frac{\xi}{\sigma}\right)\right]}\,[1 - q(\infty)], \tag{181}$$

and the mean recurrence time

$$t_{\text{rec}} = \frac{1 - \Phi\left(\frac{\xi}{\sigma}\right) + \Phi\left(\frac{\xi_0}{\sigma}\right)}{\sqrt{-\frac{\varrho''(0)}{2\pi}}\left[\Phi'\left(\frac{\xi_0}{\sigma}\right) + \Phi'\left(\frac{\xi}{\sigma}\right)\right]}\,[1 - q_c(\infty)]. \tag{182}$$

We recall that σ^2 is proportional to the number of similar, approximately independent components, that is proportional to the "size" of the mechanical system. With this fact in mind it is an easy task to estimate the values of t_{trans} and t_{rec} for intervals (171) of physical interest. In particular we obtain the mean recurrence time of a single value $\xi = \xi_0$

$$t_{\text{rec}} = \frac{\pi}{\sqrt{-\varrho''(0)}} \exp\left\{\frac{1}{2}\frac{\xi^2}{\sigma^2}\right\}[1 - q_c(\infty, \xi)]. \tag{183}$$

According to the Cramér-Khinchin representation theorem for the correlation coefficient

$$\varrho(t) = \int_{\infty}^{+\infty} \exp\{i\lambda t\}\, d_\lambda F(\lambda),\ \lim_{\lambda \to -\infty} F(\lambda) = 0,\ \lim_{\lambda \to +\infty} F(\lambda) = 1, \tag{184}$$

where the spectral distribution $F(\lambda)$ is uniquely determined by $\varrho(t)$. In particular, in our case

$$\varrho'(0) = \int_{\infty}^{-\infty} i\lambda \, d_\lambda F(\lambda) = 0, \tag{185}$$

$$\varrho''(0) = -\int_{-\infty}^{\infty} \lambda^2 \, d_\lambda F(\lambda). \tag{186}$$

Hence we find that

$$\frac{\sqrt{-\varrho''(0)}}{\pi} = \frac{\left[\int \lambda^2 \, d_\lambda F(\lambda)\right]^{\frac{1}{2}}}{\pi} = \bar{\nu} \tag{187}$$

has the character of an average frequency, and the expression for γ can be written

$$\gamma = \bar{\nu} \frac{\exp\left\{-\frac{\xi_0^2}{\sigma^2}\right\} + \exp\left\{-\frac{\xi^2}{\sigma^2}\right\}}{\Phi\left(\frac{\xi}{\sigma}\right) + \Phi\left(\frac{\xi_0}{\sigma}\right)}. \tag{189}$$

In general we can not expect that the sets of the type (171) are transitory. On the other hand it is not possible to discuss this question without a knowledge of *all* the structure functions corresponding to arbitrary series of measurements of the observable represented by x (168). Assuming a Gaussian form for all these structure functions we can obtain a sufficient condition by reference to a theorem of Grenander [Grenander, 1950], which states that a Gaussian stochastic process with continuous correlation $\varrho(t)$ is metrically transitive exactly when the spectral distribution $F(\lambda)$ is continuous, that is if there are no discrete frequencies. Hence we find in particular that all sets of the form (171) are transitory if the function $F(\lambda)$ is continuous, but this condition is obviously not necessary.

6. On ergodicity and irreversibility

The phase space structure (85) consisting of the space Ω, the class $\mathfrak{F}$ of measurable subsets of Ω, the invariant measure $\mu(\,.\,)$ the kinetic transformation u, and the time reversal transformation τ, has been constructed as a framework for the description of all possible observable events occurring in the series of measurements of the observables A (3). The measurable subsets of Ω correspond uniquely (within μ-equivalence) to the observable events. In order to meet the needs of logic the class $\mathfrak{F}$ has to be closed under the elementary set operations (taking the complement, formation of denumerable unions and intersections; in the terminology of integration theory, $\mathfrak{F}$ is a sigma-field). As the phase space structure (85) has the same fundamental properties as the phase space of a classical mechanical system, the developments of section 3.1 are applicable also to Ω. The (measurable) complex functions of the phase represent the macroscopic observables associated with the experiment considered. The linear operators on phase functions which correspond to u and τ are defined as in 3.1

$$U\,x(\omega)=x(u\,\omega), \tag{190}$$

$$T\,x(\omega)=x(\tau\,\omega). \tag{191}$$

A subclass of all complex functions of the phase is formed by the functions invariant under U. This class is obviously linear, that is closed under addition and multiplication by complex numbers, and invariant under the time reversal operation T as

$$U\,x=x \quad \text{implies} \quad U\,T\,x=T\,x. \tag{192}$$

The U-invariant phase functions represent the integrals of the macroscopic motion. The assignment of numerical values to all the integrals of the macroscopic motion, that is to all invariant phase functions, is equivalent to a prescription of the macroscopic conditions under which the series of measurements of the observables A is carried out. As a consequence of the macroscopic nature of the observables A the number of functionally independent integrals of the macroscopic motion will usually be small. That is, we expect that the macroscopic constraints can be characterized by a small number of real parameters:

$$B=(B_1, \ldots, B_n). \tag{193}$$

We have given here a somewhat heterodox formulation of the ergodic problem in statistical mechanics. We recapitulate the essential points. We consider as given the structure of the mechanical system and the phase functions or operators which represent the macroscopic observables A. Hence the phase space structure (85) corresponding to all possible observations of the system through measurements of the observables A, is determined. The integrals of the macroscopic motion are the parameters which determine the macroscopic conditions under which a particular observation series is carried out. The ergodic problem, as we consider it, is the coordination of macroscopic observables and integrals of the macroscopic motion. By definition a particular experiment is always carried out with the values of the macroscopic integrals of the motion fixed. The values may of course be unknown to the observer, and the purpose of his experiment may be a determination of them.

The integrals of the macroscopic motion and the measure $\mu(.)$ determine a conditional measure $\mu^B(.)$ in Ω corresponding exactly to the conditional measure induced by the Liouville measure on the energy surfaces in classical mechanics. The technical details of the construction of the conditional measure $\mu^B(.)$ will not be given here. The problem is intimately connected with the probabilistic concept "sufficient statistic", see [Halmos and Savage, 1949], and also [von Neumann, 1932] (in particular p. 617). For the description of the experiment discussed above we may thus restrict ourselves to one "ergodic surface" of the phase space, corresponding to fixed values of the integrals B of the macroscopic motion. The induced measure $\mu^B(.)$ on this "surface" is u-invariant. According to its construction the decomposition of the phase space Ω into "ergodic surfaces" is minimal, in the sense that no further decomposition into invariant parts can be obtained. In the following we shall restrict ourselves to one particular "ergodic surface". For simplicity we use the notation (85) for the corresponding induced phase space structure and assume that, the induced measure is finite

$$0 < \mu(\Omega) < +\infty. \tag{194}$$

This condition is satisfied in all applications of physical interest, as the macroscopic energy will always be one of the integrals of the macroscopic motion. The finiteness of $\mu(.)$ is then a consequence of the basic assumption contained in equation (1).

We observe that the reduced phase space structure corresponding to one "ergodic surface" will contain the time reversal transformation τ only if the integrals of the macroscopic motion are invariant under T.

We can now apply Birkhoff's ergodic theorem which states that under the given conditions the time-average of any phase function exists and is equal to the corresponding phase average

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} x(u^k \omega) = \frac{\int x(\omega)\, \mu(d\omega)}{\mu(\Omega)}. \tag{195}$$

We recall that every phase function $x(\omega)$ represents a macroscopic observable associated with the experiment discussed above and that the phase average is taken over a "surface" determined by given values of the integrals of the macroscopic motion. However Birkhoff's theorem is an asymptotic statement. It is physically important to know how fast the convergence of the time average to the phase average is for particular macroscopic observables. Questions of this kind are conveniently studied with the aid of the spectral resolution of the operator U restricted to the Hilbert space of all phase functions whose square is integrable with respect to the measure $\mu(.)$.

6.1. *The spectral resolution of U. Classification of observables*

In the Hilbert space of the phase function with integrable square, conventionally denoted by $L^2(\Omega, \mu)$, the scalar product and the norm are denoted by

$$\langle x | y \rangle = \int_\Omega \overline{x(\omega)}\, y(\omega)\, \mu(d\omega), \qquad \|x\| = \langle x | x \rangle^{\frac{1}{2}}. \tag{196}$$

It was first pointed out by Koopman [Koopman, 1931] that the transformation U defined by (190) is unitary. This is a simple consequence of the fact that the measure $\mu(.)$ is invariant under the point transformation u, and that this transformation has an inverse.

Assuming that the integrals of the macroscopic motion are invariant under time reversal we find by the same argument that the transformation T defined by (191) is unitary.

As U is unitary it has a spectral resolution of the form, see e.g. [Hopf, 1937],

$$U = \int_0^{2\pi} \exp\{i\lambda\}\, dE_\lambda, \tag{197}$$

where E_λ, the spectral distribution of U, is a projection valued function on the interval $[0, 2\pi]$ satisfying

$$E_\lambda E_{\lambda'} = E_{\min(\lambda,\lambda')}, \quad E_0 = 0, \quad E_{2\pi} = I, \quad E_{\lambda-0} = E_\lambda, \tag{198}$$

and the integral (197) is to be understood in the sense that for arbitrary x, y in $L^2(\Omega, \mu)$

$$\langle x | U | y \rangle = \int_0^{2\pi} \exp\{i\lambda\} \, d_\lambda \langle x | E_\lambda | y \rangle, \tag{199}$$

the integral (199) being an ordinary Stieltjes' integral.

A conjugation operation J can be defined in $L^2(\Omega, \mu)$ by

$$J x(\omega) = \overline{x(\omega)}. \tag{200}$$

Both the transformations U and T are real in the sense that they commute with the conjugation operation J. For the spectral distribution of U this commutation implies the symmetry

$$J E_\lambda J = I - E_{(2\pi-\lambda)+0}. \tag{201}$$

The commutation relation for U and T, expressing time reversal invariance,

$$T U T = U^{-1}, \tag{202}$$

gives rise to a relation similar to (201)

$$T E_\lambda T = I - E_{(2\pi-\lambda)+0}. \tag{203}$$

The spectral distribution E_λ of U induces a decomposition of the Hilbert space into three mutually orthogonal subspaces, whose projections

$$E^a, \; E^{sc}, \; E^{sd}; \quad E^a + E^{sc} + E^{sd} = I, \tag{204}$$

are compatible with E_λ, and are such that

$$E_\lambda = E^a E_\lambda + E^{sc} E_\lambda + E^{sd} E_\lambda \tag{205}$$

is a decomposition of E_λ into an absolutely continuous part, a singular continuous part, and a singular discrete part (the eigenvalue part) with respect to the Lebesgue measure in $[0, 2\pi]$.[1] E^{sd} is the projection on $L^2(\Omega, \mu)$ onto the subspace spanned by all eigenvectors of U. If x is an arbitrary element in $L^2(\Omega, \mu)$ we have the decomposition of the distribution function on $[0, 2\pi]$

$$\langle x | E_\lambda | x \rangle = \langle x | E^a E_\lambda | x \rangle + \langle x | E^{sc} E_\lambda | x \rangle + \langle x | E^{sd} E_\lambda | x \rangle \tag{206}$$

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[1] The proof of the decomposition into a continuous and a discrete part is given in most texts on functional analysis. A proof of the decomposition into a singular and an absolutely continuous part can be found in [Uhlhorn, 1960 b].

into three parts, the first distribution function being equal to the integral of a density function, the second being continuous with derivative zero and the third being a jump function, the jumps corresponding to eigenfrequencies of U. The different parts of the spectral distribution may be said to express various degrees of irreversibility (see below). It is an easy task to show that the decomposition (204) is compatible with the operation J and with the operator T, hence the orthogonal decomposition of the Hilbert space corresponding to (204) is invariant under J and under T, and the symmetry relations (201) and (202) hold for each part of the spectral distribution if in the formulae the unit operator I is replaced by the projection onto the corresponding subspace. In particular one finds that the eigenfrequencies occur in pairs $(\lambda, -\lambda)$.

The ergodic theorem of von Neumann can be stated in the form: For arbitrary x in $L^2(\Omega, \mu)$ the time average exists and is equal to a U-invariant element

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{n=N-1} U^n x = E_{+0} x. \tag{207}$$

Here E_{+0} is according to the definition of E_λ equal to the projection onto the subspace of eigenvectors of U corresponding to the eigenfrequency 0, that is the subspace of U-invariant elements. This subspace is also J- and T-invariant and in particular contains the normalized element e

$$e(\omega) \equiv \mu(\Omega)^{-\frac{1}{2}}, \quad \langle e | e \rangle = 1 \tag{208}$$

which spans the subspace of constant phase functions. The phase average of an arbitrary element x is evidently equal to

$$e \langle e | x \rangle. \tag{209}$$

In the following we give a classification of the observables according to their "degree of irreversibility".

Ergodic element

Let an element x be called ergodic if the time average (207) and the phase average (209) are equal, that is if

$$E_{+0} x = e \langle e | x \rangle, \tag{210}$$

or equivalently if its spectral distribution $\| (E_\lambda - |e\rangle\langle e|) x \|^2$ has no jump at $\lambda = 0$. We have already assumed that the transformation u is metrically transitive, or equivalently that the only invariant functions are the constant functions, hence in our particular case every element is ergodic. The criterion for ergodicity may be written

$$E_{+0} = |e\rangle \langle e|. \tag{211}$$

Ergodic event

An event Δ (subset of the phase space) will be said to be ergodic if the corresponding indicator function $I(\Delta, \omega)$ ($I(\Delta, \omega) = 1$ if $\omega \in \Delta$, $= 0$ if $\omega \notin \Delta$) is an ergodic element. We find immediately that the complementary set of an ergodic set must be ergodic and transitory according to the definition of section 5. Hence the simplified expression for the mean recurrence time applies to an ergodic set.

Weakly mixing element

Let an element x be called weakly mixing if $x - e\langle e|x\rangle$ does not belong to the subspace spanned by the eigenvectors of U, that is

$$(E^a + E^{sc})\,x = x - e\,\langle e\,|\,x\rangle, \tag{212}$$

or equivalently if its spectral distribution $\|(E_\lambda - |e\rangle\langle e|)\,x\|^2$ is a continuous function of λ in $[0, 2\pi]$.

Criteria

1. An element x is weakly mixing if and only if

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{n=N-1} |\langle x|U^n|x\rangle - \langle x|e\rangle\langle e|x\rangle| = 0. \tag{213}$$

2. An element x is weakly mixing if and only if there exists a set $J(x)$ of positive integers such that $J(x)$ has density zero and such that if n is restricted to be outside $J(x)$, then

$$\lim_{\substack{n\to\infty\\ n\notin J(x)}} \langle x|U^n|x\rangle = \langle x|e\rangle\langle e|x\rangle. \tag{214}$$

To say that $J(x)$ has density zero means that the ratio of the number of those integers between 0 and $n-1$ that belong to $J(x)$ to the total number, that is n, tends to zero as n tends to infinity.

The proofs of these criteria can be extracted from [Halmos, 1956]. For the following definitions compare also [Hopf, 1937].

Weakly mixing event

An event Δ will be said to be weakly mixing if the corresponding indicator function $I(\Delta, \omega)$ is a weakly mixing element. In particular we have, using the second criterion above

$$\lim_{\substack{n\to\infty\\ n\notin J(\Delta)}} \frac{\mu(\Delta \cap u^{-n}\Delta)}{\mu(\Omega)} = \left[\frac{\mu(\Delta)}{\mu(\Omega)}\right]^2. \tag{215}$$

Evidently the complementary set of Δ is weakly mixing with Δ.

Strongly mixing element

Let an element x be called strongly mixing if

$$\lim_{n\to\infty} \langle x|U^n|x\rangle = \langle x|e\rangle\langle e|x\rangle. \tag{216}$$

Sufficient condition

In order that an element x be strongly mixing it is sufficient that $x - e\langle e|x\rangle$ belongs to the absolutely continuous part of the spectral distribution of U, that is

$$E^a x = x - e\langle e|x\rangle, \tag{217}$$

or equivalently that the spectral distribution of x, $\|(E_\lambda - |e\rangle\langle e|)x\|^2$ is absolutely continuous, i.e. has a density.

Strongly mixing event

An event Δ will be said to be strongly mixing if the corresponding indicator function $I(\Delta, \omega)$ is a strongly mixing element. Applying (216) to $I(\Delta, .)$ we find the condition

$$\lim_{n\to\infty} \frac{\mu(\Delta \cap u^{-n}\Delta)}{\mu(\Omega)} = \left[\frac{\mu(\Delta)}{\mu(\Omega)}\right]^2, \tag{218}$$

illustrating the asymptotic independence of the events Δ and $u^{-n}\Delta$. Obviously the complementary set of Δ is strongly mixing with Δ.

Evidently a strongly mixing element (event) is weakly mixing and a weakly mixing element (event) is ergodic. We note in particular that the defined classes are linear. Further, in physical applications we are not likely to meet spectral distributions of the singular continuous type and hence the concept weakly mixing will not occur in our discussion of the connection between irreversibility and the properties of the spectral distribution of U.

Let Δ be a strongly mixing event and Δ_1 an arbitrary event. In analogy to (218) we find

$$\lim_{n\to\infty} \frac{\mu(\Delta_1 \cap u^{-n}\Delta)}{\mu(\Omega)} = \frac{\mu(\Delta_1)}{\mu(\Omega)}\,\frac{\mu(\Delta)}{\mu(\Omega)}. \tag{219}$$

Here we may interpret

$$P(\Delta_1) = \frac{\mu(\Delta_1)}{\mu(\Omega)} \quad \text{and} \quad P(\Delta) = \frac{\mu(\Delta)}{\mu(\Omega)}$$

as the stationary probabilities of the events Δ_1 and Δ, and

$$P(\Delta_1 \cap u^{-n}\Delta) = \frac{\mu(\Delta_1 \cap u^{-n}\Delta)}{\mu(\Omega)}$$

as the probability of observing the event Δ_1 at $t=0$ and the event Δ at $t=n$. The relation (219) simply expresses the fact that the dependence between Δ_1 and Δ is lost for large time differences. Such expressed the probabilities refer to fluctuations in a system at macroscopic equilibrium. However, (219) rewritten in the form

$$\lim_{n\to\infty} \frac{P(\Delta_1 \cap u^{-n}\Delta)}{P(\Delta_1)} = P(\Delta), \tag{220}$$

expresses the approach to the equilibrium distribution of the conditional probability $\frac{P(\Delta_1 \cap u^{-n}\Delta)}{P(\Delta_1)}$. The existence of at least one, and hence of two, non trivial, mixing events, Δ and $\complement\Delta$, hence gives rise to a certain stirring in Gibbs' sense, for introducing an initial probability distribution $P_0(.)$ in Ω by

$$P_0(\Delta_1) = f_1 \mu(\Delta \cap \Delta_1) + f_2 \mu(\complement\Delta \cap \Delta_1) \qquad (\Delta_1 \text{ arbitrary } \subset \Omega,\ f_1, f_2 \geqslant 0), \tag{221}$$

we have

$$P_n(\Delta_1) = P_0(u^{-n}\Delta_1), \tag{222}$$

and from (219), (220) the asymptotic form for any such distribution

$$\lim_{n\to\infty} P_n(\Delta_1) = P(\Delta_1) \tag{223}$$

is seen to be the uniform distribution. If Δ and hence $\complement\Delta$ are only ergodic one has instead of (223) the weaker statement

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{n=N-1} P_n(\Delta_1) = P(\Delta_1). \tag{224}$$

One could be inclined to think that the existence of strongly mixing events is necessary for the irrreversible appearance of physical systems. That this is not so can be seen immediately from a study of the eigenvalue spectrum of the transformation U.

The eigenvectors of U

We have assumed that the point transformation u is metrically transitive, or equivalently that the vector e (208) is the unique (up to an arbitrary phase factor) normalized eigenvector of U corresponding to the eigenfrequency 0. U may have additional eigenvectors

$$U x_\lambda = \exp\{i\lambda\} x_\lambda,\ \langle x_\lambda | x_\lambda \rangle = 1 \qquad (\lambda \neq 0,\ \text{real}). \tag{225}$$

As was noticed by Koopman [Hopf, 1937] it follows from the distributive property (44) of U that the function

$$\overline{x_\lambda(\omega)}\, x_\lambda(\omega) \not\equiv 0 \tag{226}$$

is invariant under u and hence equal to a positive constant. Hence the corresponding normalized eigenvector can be written

$$e \cdot \exp\{i\theta_\lambda\}, \qquad (\theta_\lambda(\omega)\ \text{real}). \tag{227}$$

It follows further that if λ_1, λ_2 and λ are eigenfrequencies of u

$$U \exp\{i\theta_{\lambda_1} \pm i\theta_{\lambda_2}\} = \exp\{i(\lambda_1 \pm \lambda_2)\} \exp\{i\theta_{\lambda_1} \pm i\theta_{\lambda_2}\}; \tag{228}$$

$$U T \exp\{i\theta_\lambda\} = \exp\{-i\lambda\} T \exp\{i\theta_\lambda\}. \tag{229}$$

As direct consequences of (228), see [Halmos, 1956], the eigenvalues cannot be degenerated and with two eigenfrequencies λ_1 and λ_2 also $\lambda_1+\lambda_2 \pmod{2\pi}$ and $\lambda_1-\lambda_2 \pmod{2\pi}$ are eigenfrequencies. Hence it follows from (229) that

$$T \exp\{i\,\theta_\lambda\} = \exp\{-i\,\theta_\lambda\} \tag{230}$$

or

$$\theta(\tau\,\omega) = -\theta(\omega) \qquad (\mathrm{mod}\ 2\pi), \tag{231}$$

an expression of the trivial fact that the "angular variables" $\theta(\omega)$ are odd with respect to time reversal.

For the physical application it is important that the eigenfrequency spectrum of U is either of the form

$$\lambda_n = n\,\lambda_0 \ (\mathrm{mod}\ 2\pi) \qquad (\lambda_0 > 0;\ n = 0,\ \pm 1,\ \pm 2, \dots) \tag{232}$$

where λ_0 is the smallest positive eigenfrequency, or the eigenfrequencies form a point set which is dense on the unit circle, or the eigenfrequency spectrum contains only the point 0. In the first case the angular variables are all generated by a single function

$$\theta_{\lambda_n}(\omega) = n\,\theta_{\lambda_0}(\omega) \ (\mathrm{mod}\ 2\pi). \tag{233}$$

If the corresponding eigenvectors span the space $L^2(\Omega, \mu)$, the system is obviously equivalent to a one-dimensional harmonic oscillator in classical mechanics. This case is not likely to occur in a phase space structure generated by macroscopic observables. On the other hand a *sufficient* condition for the second case to occur is the existence of at least two rationally independent eigenfrequencies, λ_1 and λ_2:

$$m\,\lambda_1 + n\,\lambda_2 = 0 \qquad (m,\ n,\ \text{integer})\ \text{implies}\ m = n = 0. \tag{234}$$

The uniform distribution of the eigenfrequencies of U over the unit circle which is a consequence of the Koopman-property (44) is remarkable. As we have seen we can expect that except for singular cases the eigenfrequency spectrum, if not empty, will be dense on the unit circle. Whether the continuous spectrum of U has similar uniformity properties or not is not known, though from physical reasons it seems likely to be the case. It seems plausible that the spectrum of a transformation U corresponding to macroscopic observables has no gaps.

Consider an element x representing an observable and assume that the phase average of x, $e\langle e|x\rangle$, is equal to zero. Then $\varrho(n) = \dfrac{\langle x|U^n|x\rangle}{\langle x|x\rangle}$ is the correlation function of the "stochastic process" $x_n = U^n x$, and is an expression for the stochastic dependence between x_t and x_{t+n}

$$\varrho(0) = 1, \quad |\varrho(n)| \leqslant 1. \tag{235}$$

If in particular x is mixing the value of the correlation function $\varrho(n)$ tends to zero with increasing n. However, completely generally we have from the spectral resolution of U (197) the Cramér-Khinchin representation of $\varrho(n)$

$$\varrho(n) = \int_0^{2\pi} \exp\{i\lambda n\}\, dF(\lambda) = \int_0^{2\pi} \exp\{i\lambda n\}\, d_\lambda \frac{\langle x | E_\lambda | x\rangle}{\langle x | x\rangle}. \tag{236}$$

The ergodicity of the element x can also be expressed by (compare (210))

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{n=N-1} \varrho(n) = 0. \tag{237}$$

It is easily seen that if the eigenfrequency spectrum of U is dense on the unit circle we can find elements x with an arbitrary prescribed form of the correlation function within any time interval of finite length. If further the absolutely continuous part of the spectral resolution of U has no gaps we can reject the requirement that the time interval be of finite length. In this sense we can obtain "approach to equilibrium" within any required degree of approximation.

Gaussian approximation

In many cases of physical interest it may be admissible to assume that a stationary stochastic process $x_n = U^n x$ corresponding to a macroscopic observable is approximately Gaussian, though it may be very difficult to give a formal proof of the fact, except for very special cases. Under this assumption the process is completely determined by its correlation function $\varrho(n)$ and in particular the stochastic process is metrically transitive (ergodic) if and only if the spectral distribution of $\varrho(n)$ (237) is continuous [Grenander, 1950]. It can easily be seen that for a Gaussian process the concepts metric transitivity and weak mixing are equivalent. Further, if the spectral distribution (237) is absolutely continuous, that is possesses a density, or more generally if $\varrho(n) \to 0$ for $n \to \infty$, the Gaussian process will be strongly mixing. An elementary proof of the last propositions can be obtained by consideration of elements of the form

$$y(k;\, \omega) = \exp\left\{i\, k \frac{x(\omega)}{\|x\|}\right\} \qquad (k \text{ real}). \tag{238}$$

From the assumption about x it follows that

$$\langle y(k') | U^n | y(k)\rangle = \exp\{-\tfrac{1}{2}[k^2 + k'^2 + 2kk'\varrho(n)]\}, \tag{239}$$

and hence if for $n \notin J$ (J of density zero), $\lim_{n\to\infty} \varrho(n) = 0$, (compare (214)),

$$\lim_{\substack{n\to\infty \\ n\notin J}} \langle y(k') | U^n | y(k)\rangle = \langle y(k') | e\rangle \langle e | y(k)\rangle \tag{240}$$

which expresses the fact that each $y(k)$ is a weakly mixing element. It follows from the fact that the weakly mixing elements form a subspace that the subspace generated by all finite products of the form

$$\prod_k U^{n_k} y(k) \qquad (n_k \text{ integer}) \tag{241}$$

is contained in the subspace of weakly mixing elements. However, the elements of the form (241) generate the complete Hilbert space $L^2(\Omega, \mu)$ of the stochastic process and hence the process is weakly mixing according to the definition of [Hopf, 1937]. Similarly if $\lim_{n\to\infty} \varrho(n) = 0$, without restriction, it follows that (240) holds without restriction, that is $y(k)$ is a strongly mixing element for each k. Hence it follows as above that any element of the Hilbert space of the stochastic process is strongly mixing and the process is strongly mixing in the terminologi of [Hopf, 1937].

These results can be extended to multidimensional Gaussian processes without difficulty.

APPENDIX

Simplified derivation of the mean transition time

Consider an incompressible stationary flow in the phase space Ω. Let Δ be a phase region of finite measure $\mu(\Delta)$ and let $J(\Delta)$ be the *total* flow into Δ in the unit of time = total flow out of Δ in the unit of time (incompressibility). Those points which enter Δ in the interval dt are said to form the front (Gibbs' terminology). The measure of the front is $J(\Delta)\,dt$. We want to determine the mean of the times which the points of the front spend in Δ = mean transition time $t(\Delta)$.

If in particular Δ is a tube of flow of finite length all points of the front have the same transition time $t(\Delta)$, if differences of the order dt are neglected, and we have the relation

$$\mu(\Delta) = T(\Delta)\,J(\Delta). \tag{A 1}$$

If Δ can be decomposed into several disjoint tubes of flow, $\mu(\Delta) = \sum_i \mu(\Delta_i)$ in such a way that $J(\Delta) = \sum_i J(\Delta_i)$ we find

$$T(\Delta) = \frac{\sum_i dt\,J(\Delta_i)\,T(\Delta_i)}{\sum_i dt\,J(\Delta_i)} = \frac{\sum_i \mu(\Delta_i)}{\sum_i J(\Delta_i)} = \frac{\mu(\Delta)}{J(\Delta)}. \tag{A 2}$$

An arbitrary phase region Δ can be decomposed into two disjoint parts Δ' and Δ'' such that Δ' is the sum of a number of tubes of flow as described above and Δ'' consists of all the points in Δ which remain in Δ forever, that is $J(\Delta'') = 0$. Hence we have for an arbitrary phase region

$$T(\Delta) = \frac{\mu(\Delta')}{J(\Delta')} = \frac{\mu(\Delta)}{J(\Delta)} \cdot \frac{\mu(\Delta - \Delta'')}{\mu(\Delta)}, \tag{A 3}$$

where the second factor represents the "probability" that a point chosen "at random" in Δ will leave Δ within a finite time.

It is possible to make this derivation rigorous.

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